

Conductance through a One-Dimensional Correlated System: Relation to Persistent Currents and Role of the Contacts

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Based on a recent proposal [O.P. Sushkov, Phys. Rev. B **64**, 155319 (2001)], we relate the quantum conductance through a sample in which electrons are strongly correlated to the persistent current of a large ring, composed of the sample and a non-interacting lead. A scaling law in the lead length allows to extrapolate to a well-defined value of the conductance, depending only on intrinsic properties of the sample and the nature of the contacts between the sample and the lead. For strongly disordered samples, the conductance is found to be enhanced by the interaction.

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Viewing quantum transport as a scattering problem [1, 2] generated a new understanding of the electronic conductance. This approach is able to explain a wealth of experimental results [3] in mesoscopic systems when electron-electron (e-e) correlations are not important. To include these correlations is non-trivial and remains one of the major challenges in the field (see e.g. [4]). While none of the proposals to calculate the conductance for a correlated system is well suited for numerical calculations [5, 6] or free of certain assumptions [7], such an issue becomes crucial in present day's research exploring electronic transport through nanosystems (carbon nanotubes [8], molecules [9], and point contacts [10]), where the Coulomb repulsion leads to important correlations.

Reservoirs and leads are key elements in the scattering approach, and possess very clear physical meanings since the measurement is made with electrodes which behave as electron reservoirs. In a good electrode, the electron density n_e is large, the ratio r_s between Coulomb and Fermi energy is small, hence the e-e interaction is negligible. In contrast, n_e in a nanosample can be very small, yielding a large ratio r_s and important e-e correlations.

The dimensionless conductance g does not only depend on the intrinsic properties of the sample, but also on the way it is connected to the electrodes. The quality of the contacts is particularly important for correlated electrons. For a clean Luttinger liquid attached to non-interacting leads through reflectionless contacts, it has been found [11] that the interactions do not influence g . In the other extreme, if the contacts are tunnel barriers, the interactions lead to Coulomb blockade [12], thereby dominating g . In carbon nanotubes, various transport regimes are observed depending on the nature of the contacts [8].

As shown by Kohn [13] and Thouless [14], g is also related to the sensitivity of the sample's eigenstates to a change of the boundary conditions. This sensitivity

can be tested by closing a system to a ring and measuring the persistent current as the response to an enclosed magnetic flux ϕ . At zero temperature, the persistent current is given by $J = -\partial E/\partial\phi$, where E is the ground state energy of the many-body system. Interactions play an important role for J , and it is generally accepted that they account for the large difference between experiments and one-particle calculations [15]. There have been various attempts [7, 16] to link J and g for an interacting ring. However, the ring built from the sample itself does not contain any reservoirs in which energy relaxation can take place. Negative zero-frequency conductivities occur [17], unlike in the dissipative case in which we are interested here.

As pointed out in Refs. [5, 10], at zero temperature, not only for the non-interacting case, but also for correlated samples, g is given by $|t(E_F)|^2$, the probability for an electron at the Fermi energy E_F to be elastically transmitted through the sample. Moreover, if one replaces the massive electrodes (with negligible e-e correlations) used in a real measurement by very long non-interacting one-dimensional leads, one can expect that they have a similar effect [6]. Sushkov recently proposed [10] that $|t(E_F)|^2$ can be extracted from the persistent current of a much larger ring, composed of the sample itself, together with a long lead closing the system. This has the considerable advantage that a ground state property (J) suffices to determine g . However, one needs the J of the *combined system* (sample plus lead), and not the one of the system alone as in previous works [7, 13, 14, 16].

In the following, we adapt the approach of Ref. [10] to calculate g for one-dimensional interacting electrons using the Density Matrix Renormalization Group (DMRG) algorithm [18, 19]. We check that a scaling law allows to extrapolate to an infinite lead, yielding g as a property of the sample and the way it is connected to the lead. The nature of the contacts turns out to play a major

role. Then, we extend our analysis to disordered samples, where we find that, similarly to the case of persistent currents [20], repulsive interactions may increase g for strong disorder.

We first present an alternative derivation of Sushkov's result [10], pointing out the main assumptions, for the non-interacting case. As depicted in the upper inset of Fig. 1, we consider a sample (S, hashed region) closed to a ring by a non-interacting and disorder-free lead (L), and threaded by a flux ϕ . The total length $L = L_S + L_L$ consists of the sample length L_S and the lead length L_L . The one-particle eigenstates of the total system satisfy

$$\det(I - M_S M_L) = 0, \quad (1)$$

with the transfer matrices of the sample and the lead

$$\begin{aligned} M_S &= \frac{1}{\sin \varphi} \begin{pmatrix} e^{i\alpha}/\sin \theta & -i \cot \theta + \cos \varphi \\ i \cot \theta + \cos \varphi & e^{-i\alpha}/\sin \theta \end{pmatrix} \\ M_L &= e^{i\Phi} \begin{pmatrix} e^{ikL_L} & 0 \\ 0 & e^{-ikL_L} \end{pmatrix}, \end{aligned} \quad (2)$$

respectively. Here, $\Phi = 2\pi\phi/\phi_0$ where ϕ_0 is the flux quantum. The scattering is characterized by the angle θ , the phase-shift α , and the angle φ (equal to $\pi/2$ if right-left symmetry is respected). These angles are functions of k , the wave-vector in the lead. The transmission amplitude is given by $t = e^{i\alpha} \sin \theta \sin \varphi$. With (2), the quantizing condition (1) can then be written as

$$\cos \Phi = \frac{1}{|t|} \cos(kL + \delta\alpha), \quad (3)$$

with the relative phase-shift $\delta\alpha = \alpha - kL_S$. The persistent current carried by a one-particle state (with energy ϵ) is $j(\phi) = -(\partial\epsilon/\partial k)(\partial\phi/\partial k)^{-1}$. We work at $\Phi = \pi/2$ and establish two crucial assumptions: i) $|\partial(\delta\alpha)/\partial k| \ll L$; ii) $\partial\epsilon/\partial k \simeq \hbar^2 k/m$. The first one states that the Wigner time associated with the scattering region is negligible compared with the time spent in the leads. Notice that we work with a relative Wigner time $\tau_W = (m/\hbar^2 k)\partial(\delta\alpha)/\partial k$, that is, the difference between the delay time of the scattering region and that of a potential-free region having the same length. The second assumption implies that the dispersion relation is essentially unaffected by the scattering potential.

The persistent current of N non-interacting spinless fermions (for simplicity we take N even) is given by [21]

$$J(\Phi = \pi/2) = \frac{e\hbar}{mL} k_F |t(k_F)|. \quad (4)$$

Denoting by J^0 the persistent current of a clean ring of length L , the conductance may be expressed as [10]

$$g = \lim_{L_L \rightarrow \infty} \left(\frac{J(\pi/2)}{J^0(\pi/2)} \right)^2. \quad (5)$$

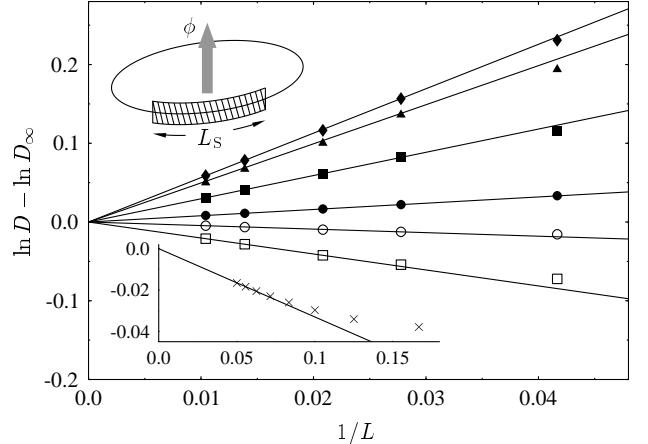


FIG. 1: Scaling of $\ln D$ with the total length L of the system, showing a linear increase of $\ln D$ with $1/L$ for even $L_S = 12$ ($U = 1$ (\bullet), $U = 2$ (\blacksquare), $U = 3$ (\blacktriangle), $U = 4$ (\blacklozenge)), and a decrease for odd $L_S = 13$ ($U = 1$ (\circ) and $U = 2$ (\square)). Lower inset: scaling for unpolarized electrons within the Hubbard model ($L_S = 2$, $U = 1$). Upper inset: sketch of a ring consisting of the sample (hashed region) and a non-interacting lead threaded by a flux ϕ .

With interaction [22], assumptions i) and ii) always hold in the large L limit. Moreover, the use of Eq. (5) implies that the one-particle states of the correlated system can still be indexed by the lead wave-vectors k . That is, adding an infinite non-interacting lead to a finite non Fermi-liquid sample restores the Fermi-liquid behavior. This assumption, which has been used in the perturbative calculation of transport through Hubbard chains connected to reservoirs [23], requires that the interactions are *completely* switched off in the one dimensional lead. Otherwise the Luttinger liquid behavior [24] sets in, and one cannot obtain a result which is independent of the length of the auxiliary lead. In this, our approach differs from Sushkov's, where the interactions in the lead are kept (within the Hartree-Fock approximation).

Eq. (5) allows to calculate g from ground-state energies. We do this for spinless fermions (polarized electrons) in a ring described by the Hamiltonian

$$H = - \sum_{i=1}^L (c_i^\dagger c_{i-1} + c_{i-1}^\dagger c_i) + \sum_{i=2}^{L_S} U \left[n_i - \frac{1}{2} \right] \left[n_{i-1} - \frac{1}{2} \right] \quad (6)$$

where c_i (c_i^\dagger) is the annihilation (creation) operator at site i , $n_i = c_i^\dagger c_i$ the number operator, and the flux-dependent boundary condition enters through $c_0 = \exp(i\Phi)c_L$. The interaction is restricted to nearest neighbors and effective in the sample, but vanishing in the lead. It is equilibrated by a compensating potential that prevents the particles from emptying the interacting region. The form of the Hamiltonian allows to have

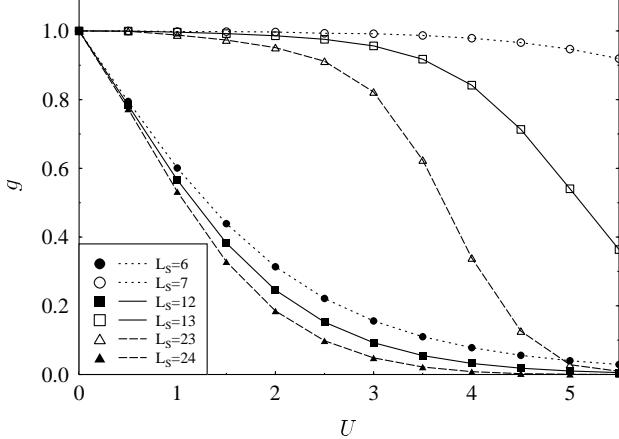


FIG. 2: Conductance g as a function of the interaction strength U for different values of the sample length L_S .

particle-hole symmetry at half filling. We work with a number of fermions $N = L/2$, such that the mean density is always $1/2$ independently of L_S and L_L .

Using the DMRG algorithm as described in Ref. [19], we calculate the ground-state energies $E(\Phi)$ at $\Phi = 0$ and $\Phi = \pi$, to obtain the stiffness $D = (L/2)|E(0) - E(\pi)|$ (which is simpler to calculate than J). When the flux-dependence of the ground-state energy is sinusoidal, which is the case in one-dimensional localized systems, D is directly proportional to the maximum J . We will use such an identification to calculate g from Eq. (5), taking D instead of J [22].

An obvious requirement for Eq. (5) to be useful is that the resulting g should be independent of L_L , since the lead is an auxiliary element of the procedure. Therefore, the first numerical step is to compute D for increasing L_L with given L_S and U (Fig. 1). We find a very clear asymptotic behavior, described by the scaling law

$$D(U, L_S, L_L) = D_\infty(U, L_S) \exp\left(\frac{C(U, L_S)}{L}\right), \quad (7)$$

where the *intrinsic value* D_∞ is *independent* of the length of the auxiliary lead. This asymptotic value D_∞ is then used to determine the conductance as $g = (D_\infty/D_\infty^0)^2$, where D_∞^0 corresponds to the clean non-interacting ring. The sign of C [25] depends on the parity of the number of sites L_S in the sample: $C > 0$ for even L_S (filled symbols) and $C < 0$ for odd L_S (open symbols).

The method also works for non-polarized electrons (Hubbard model with on-site interaction), and the size-scaling again allows to obtain intrinsic values (lower inset in Fig. 1). In the sequel we concentrate on the spinless case (Hamiltonian (6)), which contains the main features we are interested in, and allows to reach larger samples.

Having verified the consistency of our approach, we now study the systems of interest. In Fig. 2 we present

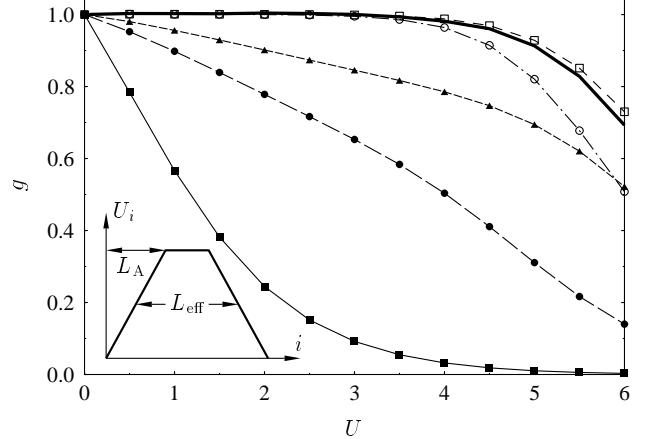


FIG. 3: Conductance g as a function of the interaction strength U , for a fixed $L_{\text{eff}} = 12$, and increasing smoothing of the contacts, defined by the length L_A (see inset). Filled (open) symbols correspond to even (odd) L_S ; $L_A = 1$ (\circ), and $L_A = 9$ (\square), $L_A = 0$ (\blacksquare), $L_A = 4$ (\bullet), and $L_A = 10$ (\blacktriangle). Using the same smoothing length ($L_A = 10$) but improving in the shape (a tanh function (thick solid line) instead of a linear increase (\blacktriangle)) helps g to approach the perfect value.

the conductance, as a function of U , for various sample lengths L_S . One observes a monotonic decrease with increasing U , and a very clear even-odd asymmetry according to the parity of L_S . Samples with odd L_S exhibit almost perfect transmission up to large values of U , while an even L_S results in a decrease of $g(U)$ already at weak interaction. For odd L_S , particle hole symmetry leads to degenerate sample configurations with $(L_S \pm 1)/2$ particles in the interacting region. This is similar to a Coulomb blockade resonance. The traveling particle can thus become trapped for a long time ($\tau_W > 0$), consistent with negative C [25]. Since the two configurations are coupled by processes which transfer particles through the interacting sample, one obtains perfect transmission, as in the perturbative treatment of Ref. [23].

On the other hand, an even number of sites implies that the transport of one particle through the sample takes place via a virtual state with an energy of order U above the ground-state. Thus, no resonance can be expected and the transmission, which is suppressed already by moderate U , is a fast process with $\tau_W < 0$, consistent with $C > 0$. In addition, increasing L_S reduces g linearly for small U , and exponentially for $U > 2$, consistent with the Mott-insulating behavior.

The even-odd asymmetry, and the perfect transmission for the odd case, point to the importance of the contacts. In order to investigate their role, we introduce a position dependent interaction strength U_i which increases linearly from 0 to its maximum value U , inside the “contacts” of length L_A (see inset of Fig. 3). As shown in

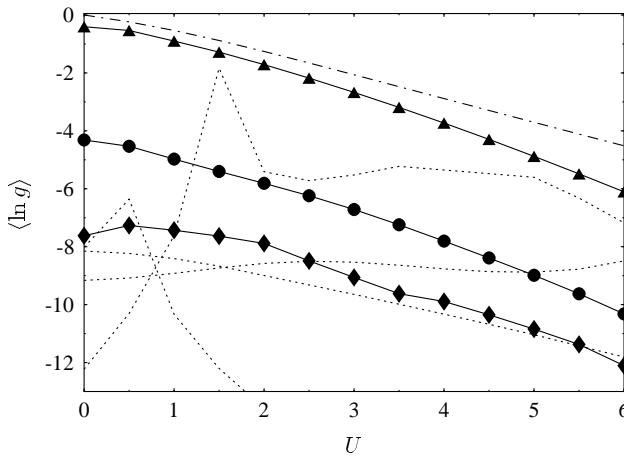


FIG. 4: Ensemble averages of $\ln g$ as a function of the interaction at $L_S = 8$, in the presence of disorder $W = 1$ (\blacktriangle), 5 (\bullet) and 9 (\blacklozenge). The statistical errors are smaller than the symbol size. The dash-dotted line represents the clean case, the dotted lines represent four individual samples at $W = 9$.

Fig. 3, these smooth contacts increase g , at constant effective length $L_{\text{eff}} = L_S - L_A$ of the sample. The effect is pronounced in the case of even L_S and the conductance approaches the ideal situation of perfect transmission expected for reflectionless contacts when we improve the smoothing [11]. While the form of the contacts preserves the right-left symmetry, the smoothing leads to an extension of the perfect transmission at odd L_S towards higher values of U . However, we found that asymmetric contacts destroy the perfect transmission. The strong influence of the contacts is crucial when describing experiments since it seems impossible to connect a nanosample via reflectionless contacts. It also shows the limitation of other approaches relating the conductance of an interacting sample to its intrinsic properties, without taking into account the way it is connected to the electrodes.

While clean interacting systems are of physical interest (*e.g.* carbon nanotubes), it is also important to consider the generic case of disordered systems. To this end, we add the term $W \sum_{i=1}^{L_S} v_i n_i$ to the Hamiltonian (6), where W is the disorder strength and the v_i are distributed equally in $[-1/2, 1/2]$. We have checked that D scales with L as before (Eq. (7)), ensuring a well-defined limiting value for g . The even-odd dependence of g disappears when disorder is introduced. The combined effect of disorder and interactions on g is shown in Fig. 4. In the ballistic regime (at $W = 1$ the mean free path exceeds L_S) the effect of W is weak at small U , and it becomes more pronounced at stronger U (when the disorder pins the Mott insulator, reinforcing the localization). At large W , g for individual samples exhibits peaks as a function of U whenever a charge reorganization occurs, similarly to the case of the D calculated without the lead [20]. Very remarkably, the ensemble average of $\ln g$ is *increased* by a

moderate repulsive U , showing the non-trivial interplay of disorder and interactions in a transport problem.

In conclusion, starting from a recent proposal [10], we have provided a well-defined procedure for calculating the conductance g of interacting one-dimensional wires, and used it to investigate correlation and disorder effects. While the interaction reduces g for spinless fermions in the presence of weak or moderate disorder, a moderate repulsive interaction increases g at strong disorder. We also determined the crucial role of the sample-to-lead contacts on the conductance.

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- [1] R. Landauer, IBM J. Res. Dev. **1**, 223 (1957).
- [2] M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986).
- [3] Y. Imry, *Introduction to Mesoscopic Physics*, Oxford University Press (New York 1997).
- [4] P. Prelovsek and X. Zotos, cond-mat/0203303.
- [5] Y. Meir and N.S. Wingreen, Phys. Rev. Lett. **68**, 2512 (1992).
- [6] H.M. Pastawski, Phys. Rev. B **44**, 6329 (1991).
- [7] R. Berkovits and Y. Avishai, Phys. Rev. Lett. **76**, 291 (1996).
- [8] P.L. McEuen, M.S. Fuhrer, and H. Park, IEEE Trans. Nanotech. **1**, 78 (2002), and references therein.
- [9] see *e.g.* Special issue on *Transport in Molecular Wires*, ed. by P. Hänggi, M. Ratner, and S. Yaliraki, Chem. Phys. **281**, pp. 111–487 (2002).
- [10] O.P. Sushkov, Phys. Rev. B **64**, 155319 (2001).
- [11] I. Safi and H.J. Schulz, Phys. Rev. B **52**, R17040 (1995).
- [12] L. Kouwenhoven *et al.*, in *Mesoscopic Electron Transport*, ed. by L.L. Sohn *et al.* (Kluwer 1997).
- [13] W. Kohn, Phys. Rev. **133**, A171 (1964).
- [14] D.J. Thouless, Phys. Rev. Lett. **39**, 1167 (1977).
- [15] U. Eckern and P. Schwab, Adv. Phys. **44**, 387 (1995).
- [16] B.S. Shastry and B. Sutherland, Phys. Rev. Lett **65**, 243 (1990).
- [17] R.M. Fye *et al.*, Phys. Rev. B **44**, 6909 (1991).
- [18] S.R. White, Phys. Rev. B **48**, 10345 (1993).
- [19] P. Schmitteckert, Ph.D. thesis, Univ. Augsburg, 1996.
- [20] P. Schmitteckert *et al.*, Phys. Rev. Lett. **81**, 2308 (1998).
- [21] H.-F. Cheung *et al.*, Phys. Rev. B **37**, 6050 (1988).
- [22] For a quantum dot in the Coulomb blockade regime [C.A. Stafford, R. Kotlyar, and S. Das Sarma, Phys. Rev. B **58**, 7091 (1998)], one obtains $g \propto J^2(\pi/2)$ and $g \propto D^2$.
- [23] A. Oguri, Phys. Rev. B **59**, 12240 (1999).
- [24] C.L. Kane and M.P.A. Fisher, Phys. Rev. Lett **68**, 1220 (1992).
- [25] In the non-interacting derivation of (5), the first correction in $1/L$ and τ_W have opposite sign. A potential well accelerates the particles leading to $\tau_W < 0$, and $C > 0$.